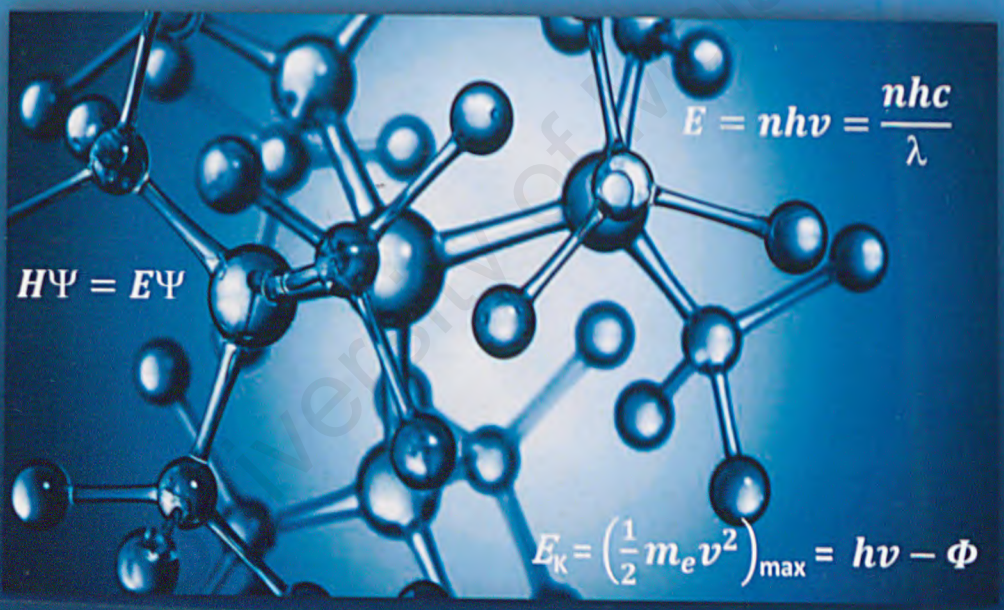
UNIVERSITY OF MALAYA

Inaugural Lecture

Some Consequences of Posing Almost Impossible Questions in the Physical Sciences



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Synopsis

Some Consequences of Posing Almost Impossible Questions in the Physical Sciences

The lecture recounts fundamental research outcomes in statistical thermodynamics, mechanics, quantum theory, thermal radiation, conductive heat transfer, variational principles and thermodynamical laws that arose from the process of posing scientific questions raised in worldwide research reported by the media. In retrospect, the object of my investigation was and is critique rectification of areas in science I was drawn to, rather than practice the safe science of gaining access into global group research endeavours served by an accrediting media, with piecemeal incremental collective development of the research topic where the fundamental assumptions were not questioned. The evidence from the citation metrics such as WOS Thomson Reuters ISI show that such type of high impact research is confined to a majority of workers in the so-called developed world supplemented by a minority of selected elites located in the periphery of the global economic pecking order, who play an iconic but usually detrimental role in their often impoverished societies due to non-sustainable irrelevance. The selected research touched upon seems to show a slow thread of continuity, where ideas that were first deduced nearly 30 years ago in statistical thermodynamics for instance only now find relevant application, for instance in the theory of heat transfer, which seems to conform to an optimized Carnot trajectory of a "recoverable conversion", mooted about 26 years back. Such a line of continuity, made possible by considerable effort also implies having to reconsider and re-assess the axiomatic concepts that safe science is not concerned with. Another driving force in this enquiry on basic research was the environment. I developed some ideas in electrochemistry and the solid state as a result of having to teach at the undergraduate level courses in these subject areas, which will be briefly outlined. None of my research conducted in UM was due primarily to international networking and organization. My extensive short term and long term

sabbatical research visits were aimed at exposure to methodologies that might aid in posing independent questions, and lately, the added intention was in gaining familiarity with standard computational tools that postgraduate and other students could use for their work. At the tail end of my work here, I became aware of the dire need of postgraduate mentoring to ensure that for the future, there could exist critical and independent work and reasoning based on passing on a tradition that one had developed, through direct personal discussion. However, due to the limitations of our students, one had to begin from a simple base and then encourage the current generation to ask their own questions within the limits of their abilities and the facilities of the supporting institution. Given the prevailing international realities, this is a difficult undertaking, due to the pressure of group collective research and its accrediting domination over personal and local interests and needs; the other difficulty is the need to protect and encourage students as they voyage into the unknown, as the costs are high, and there is also a possibility of predation of ideas and thoughts that are developed in regions that do not have the same "results" pressure of the international science bureaucracy, that also needs to create a pecking order of creativity and innovation through their press. The simple base established here with the help of a Post-Doc from India late in my career was in simple fluid state experimental studies of physicochemical and ultrasonic properties of multicomponent mixtures. Because this is a complex field, the opportunities for interpretation is very great, even for the limited educational backgrounds of many of our students. This last phase of graduate research involvement would hopefully equip me with the necessary experience to relate to the region as a whole (South and South East Asia in particular) in terms of encouraging problem solving research based on a person's own interest in part at least, which can only encourage more relevant and viable research in these fragile regions.

Some Consequences of Posing Almost Impossible Questions in the Physical Sciences

INTRODUCTION

The outline of a fraction of the results and outcomes of these almost impossible questions posed over 30 years are listed as: **[A]** Continuum thermodynamics with applications, including electrochemical systems, **[B]** Statistical thermodynamics **[C]** Foundational studies in mechanics, quantum mechanics and radiation, and **[D]** Molecular dynamics and NEMD simulations of complex systems with chemical reaction theories deduced from computer simulations and **[E]** Liquid-state laboratory for post-graduate opportunies in independent research. **[A]** describes developments in deriving minimum entropy production principles beyond Prigogine, postulating new entropy forms and derivation of Onsager reciprocity to any order with no reference to time reversal arguments. A potential theory using trivial Euler-Lagrange variations was advanced and applied to transport processes. Using the basic axioms of thermodynamics, the very influential B.C. Eu theory of an excess entropy thermodynamical function of state was disproved. Again, from basic Kelvin Clausius Second Law considerations, a new and analytically exact new diathermal entropy form was deduced for open systems. **[B]** describes a zero entropy trajectory (not connected with the Liouville equation and its coordinate space) with applications. A Brownian motion treatment of a blackbody cavity resonator shows that the Planck constant can be related to the relaxation time of the electronic oscillators lining the cavity and other related variables. Experimental consequences of this basic theory are mentioned in thermal radiation tranfer. Various phenomena in electrochemistry are examined ab initio. Various electrode capacitance and potential theorems are developed,

including another electrochemical potential of possible importance in solid state theory. **[C]** describes extensions to the Kirchoff radiation law, and proves for a common domain space, the Heisenberg uncertainty principles cannot obtain from Schrodinger wavefunctions. The central understanding of "time reversibility" as used in the physical sciences is proven to be false and is contrasted to other more legitimate definitions. Initial experiments to test the Fourier-like thermal radiation is described, and new relations for the radiancy and Kirchoff laws are postulated. Section **[D]** presents results and theories derived from MD and NEMD simulations of chemical reactions including a rationalization of the Hammet-Taft-Curtin free energy relations and the determination of the standard free energy, entropy, and enthalpy of activation from the shape profile of the molecule along its transition state reaction pathway. **[E]** Refers to work in the liquid state that has as its primary motive postgraduate opportunities for independent research. A broad area has been covered and the future goals include consolidating the outlines of the theoretical results by corroborating experimental results and by also looking to other formulations to realize possible common ground.

[A] Continuum thermodynamics with applications, including electrochemical systems

A major encouragement to attempt thermodynamical analysis based on first principle deductions, in exactly the sense of Carnot, Clausius and others in recent times came from the writings of Benofy and Quay (BQ) [1,2]. The critique of the BQ theories [3] with regard to Fourier heat conduction and thermoelectricity lead to the development of a postulate of an entropy state function and the derivation of exact thermodynamical relations for the Kelvin Heat Engine and generalized continuous alloy thermocouple and similar results obtain for analogous systems. For instance, the thermoelectric

power coefficient $\mathcal{E}(T,\mathcal{N})$ defined as the contribution to the electromotive force $\mathcal{V}$ per unit gradient of the temperature and material composition variable $\mathcal{N}$ i.e. $d\mathcal{V} = \mathcal{E}dTd\mathcal{N}$ was deduced through the Stokes theorem to have a form similar to Kelvin's second thermocouple relation, that is $\mathcal{E} = \pi/T$ where $\pi = \pi(T,\mathcal{N})$ is the reversible heat per unit charge that traverse a circuit per unit change in material composition. From the BQ reduced variable scheme, we also could derive $\mathcal{E} = \left(\frac{\partial\beta}{\partial T} - \frac{\partial\alpha}{\partial\mathcal{N}}\right)$ [4] [eq.21] where $\left.\frac{\partial\phi_e}{\partial T}\right|_{\mathcal{N}} = \alpha$ and $\left.\frac{\partial\phi_e}{\partial\mathcal{N}}\right|_{T} = \beta$. A great many new reciprocal relations were also deduced, such as

$$\frac{\partial(W'H)}{\partial\mathcal{N}}T - \frac{\partial(W'G)}{\partial T}\mathcal{N} = \pi/T \qquad (1)$$

where for internal energy Lu and potential function ϕ_e, W' is defined as $\left.\frac{\partial Lu}{\partial\phi_e}\right|_{T,\mathcal{N}}$ and $G = \frac{\partial(\phi_e)}{\partial\mathcal{N}}T$. The Kelvin engine is potentially very significant heat engine with minimal moving parts. It consists of a compressible liquid confined to a rectangular tube where two opposite ends of the rectangle are maintained at two different temperatures; the fluid circulates in this rectangular loop and could be used to do work through for example a turbine mechanism. A simplified system consists of a fluid that may be described by two variables, the density and temperature (ρ,T). Several new results pertaining to the fluid working substance may be derived, such as [4] [eq. 43]

$$\frac{\partial}{\partial\rho}(\alpha_m + \sigma_m) = \frac{\partial}{\partial T}(\beta_m + \pi_m) \qquad (2)$$

where the partials with respect to the fluid potential of the temperature and density are respectively α_m, β_m and σ_m, π_m represent the same partial derivatives with respect to the thermal transport energy. In the same paper, "conductive heat" $\mathbf{J_c}$ was defined such that $\mathbf{J_c}.\nabla T \leq 0$ is always true if the conductive heat at $\mathbf{X}$ is $\mathbf{J_c}(\mathbf{X})$ where $\mathbf{J_c}(\mathbf{X}) = \dot{Q}_{ext}$ then at a

distance $\delta\mathbf{X}$ we must have the conductive heat at this region as that due to what was dissipated out of the region $\alpha\Delta\phi\delta n$ because of degradation of the field energy to entropy, and the thermal transport energy change $dQ_H\delta n$ for amount of material δn convected, so that

$$\mathbf{J_c}(\mathbf{X}+\delta\mathbf{X}) = \dot{Q}_{ext} + \alpha\Delta\phi\delta n + dQ_H\delta n \qquad (3)$$

Since it was inferred that $Q_H\delta n/T$ was a perfect differential, it could be deduced that the entropy term $\delta S' = \sum_i^N \delta n_i X_i$ was in fact also a perfect differential leading to reciprocity in the coupling coefficients L , i.e.

$$L_{ij} = \frac{\partial\delta n_i}{\partial X_j} = \frac{\partial\delta n_j}{\partial X_i} = L_{ji} \qquad (4)$$

and indeed all other higher order L coefficients were also symmetrical. It will be remembered that the Onsager reciprocity relations (which won him the Nobel Prize) was derived from statistical mechanics using "time reversal invariance" or the principle of microscopic reversibility. which was shown to be not true [5,6]. Because [7] was written before a detailed study of mechanics was undertaken, a type of thermodynamical interpretation of "time reversibility" which does not contradict the later development was utilized to derive very general nonlinear "minimum entropy production" principles; for instance, if σ is the ordinary internal entropy production term (per unit volume) and if we define the following equations

$$\sigma' = \mathbf{J}_Q \cdot \nabla T/T^2 + \nabla\cdot(\textstyle\sum_k \mu_k \mathbf{J}_k) + \sigma \qquad (5)$$

$$\sigma'' = \sigma' - \nabla\cdot\mathbf{J}_Q^c/T \qquad (6)$$

where for (6) $\mathbf{J}_Q^c$ is the heat absorbed by the system with no associated change of state, and $\mathbf{J}_Q$ is the total heat current vector and where $\mu, \mathbf{J}_k$ are the chemical potential and species current vector, then $\sigma''_{ir}(A) \geq \sigma''_{ret}(A)$ where A is the external condition variables which are the same but where in

the case of the *ir* state, the system is relaxing to the steady state (*ret*), then we can say the the σ'' entropy tends to a minimum in constrast to Prigogine's results. The above used the postulated entropy form [7] [eq.18]

$$\oint dQ^{st,ret}/T = -\oint \nabla \cdot \mathbf{J}_Q^{st,ret}/T dt = 0 \qquad (7)$$

where $\oint dQ^{st,ret}/T \leq 0$ and which are valid for all steady states or states in transition where the superscripts define a transition about steady states along a predefined type of pathway. Within this scheme assuming the validity of the principle of local equilibrium, Prigogine's results are an approximation [3,7,4]. Jesudason [8] developed a new kind of mathematical Euler-Lagrange variational principle for so-called trivial variations together with the Noetherian conservation which may well be related to null-geodesic trajectories, and it was applied to heat conduction, diffusion and other problems in irreversible thermodynamics where all flows were expressed in terms of a single potential of form $\Phi = \sum \sum a_{ij}\phi_{ij}$. Jesudason [9,10] applied the theory of "recoverable transitions" found in [11] to a standard thermocouple circuit and it was deduced that the standard thermoelectric equations were only approximations even within the regime of the continuum and in particular the "Thomson heat" is just one term in an infinite series expansion. In time, it would be possible to test this theory against the standard ones by NEMD if suitable algorithms to deal with charge interactions could be created. This is one area of study for the future requiring first hand expertise in NEMD programming and theoretical capability. Ref. [12] is a report of a small part of what was presented in [13] concerning computational proof of changes in the electronic chemical potential of a electrode substrate, where its constancy is one assumption in electrochemistry. Ref. [14] is a significant work in the sense that it mathematically disproves as false for closed systems the influential nonequilibrium entropy definition of B.C.

Eu (who created an influential school of thermodynamics); it also proves from mathematical analysis that the principle of local equilibrium cannot rigorously hold; it is only an approximation. Jesudason [15] for the first time develops a rigourous and exact open system Carnot engine; previously people always consider closed working fluids even when considering open systems and work-transformations. This idea allowed one to come across several new state functions, in particular a new entropy function quite different from the one defined in standard open system thermodynamics where it is shown that

$$\oint \frac{dQ_{dia}}{T} = 0 \qquad (8)$$

and where the diathermal heat transfer denoted by subscript *dia* when divided by the temperature becomes a function of state, where this heat term refers to the heat absorbed by the system boundary; this implied that there exists two types of Clausius inequality, (another entropy form is $dS' = dQ_{tot}/T$ where dQ_{tot} refers to the total heat absorption) whereas in the past century and a half it was believed that a singular form existed of the form $\oint dQ_{tot}/T \leq 0$ and much of non equilibrium theory seemed to define fluxes and forces in terms of this entropy where the subscript *total* refers to an increment of the total heat absorbed; also a contradiction in the Denbigh treatment of classical entropy is mentioned. This new rigorous theory shows the B.C. Eu theory which relies on the Clausius Inequality to be open to question for open systems as well. How does one compare and contrast the above to current developments?

[B] Statistical thermodynamics

A critique of BQ [3] lead to studies in Fourier heat conduction and thermal desorption, and to a class of zero-entropy irreversible processes termed "'recoverable"' which

was developed through a new rudimentary statistical mechanics in [11] that defines a new class of entropy trajectories which are invariant along a particular non-Liouville phase-space (which was very clearly emphasized). The basic idea is that during a general "'reaction"', of a particular species, the following holds within a mean relaxation time τ

$$\widetilde{D}\delta\mathbf{\Gamma} = \widetilde{D}'\delta\mathbf{\Gamma}' \tag{9}$$

where the generalized thermodynamical space was written $\mathbf{\Gamma} = \{\mathbf{R}, \mathbf{\Omega}\}$ representing the variable spaces of the "'quantal type"' or species type and the other thermodynamical spaces respectively and $\widetilde{D}$ the density of the species concerned. The primes in eq.(9) refer to the species after a "'collision"' or discrete interaction. For simple processes where the quantal type does not change, we derive a Liouville type equation - in form only, and *not* in the Liouville space of momentum and spatial coordinates- for each quantal type N so that

$$\frac{\partial \widetilde{D}_N}{\partial t} + \nabla \cdot \left(\widetilde{D}_N \mathbf{v}\right) = 0 \tag{10}$$

or

$$\sum_N \frac{\partial \widetilde{D}_N}{\partial t} + \nabla \cdot \left(\widetilde{D}_N \mathbf{v}\right) = 0 \tag{11}$$

Furthermore, a Jacobian was introduced where $\delta\mathbf{\Gamma}' = \|J\|\delta\mathbf{\Gamma}'$ where J is the Jacobian of the transformation given variously, such as $\|J\| = (1 + \nabla \cdot \mathbf{v}dt)$. Another curious development for simple transformations is that the rate of change of the thermal entropy $\dot{S}_t$ (assuming the form $S \sim -k\sum_N \widetilde{D}_N \ln \widetilde{D}_N$ is valid for non equilibrium situations, as assumed in the H theorem) is that $\dot{S}_t \approx kk'\nabla.\mathbf{v}\sum_N \widetilde{D}'_N(\ln\widetilde{D}'_N + 1)$ where for no change in the thermal energy, $\nabla \cdot \mathbf{v} = 0$ for both equilibrium and non-equilibrium processes. It is proved that for this class of processes, the partition function remains trivially invariant. It was demonstrated that the Carnot theorem could be reduced to

local form, which stood in contradiction to the BQ statements in their consideration of both global and local processes. This theorem was applied to the problem of thermal desorption of molecules on a surface. Only recently has this idea been verified by NEMD simulations of a lattice chain, where heat conduction is shown to conform to a recoverable process. The early forays in statistical mechanics also lead to a delightfully simple theorem of relevance to irreversibility by considering the momentum impulses over the entire system [16], where it was deduced that the external work done on any general system over a short time interval τ is given by an autocorrelation function of the form (in any one dimension)

$$m\{\langle v(\tau)v(0)\rangle - \langle v^2(0)\rangle\} = \delta W \qquad (12)$$

and the above could be checked by computer simulation and seems to be uncannily related to the Diffusion type coefficients in form. It will be recalled that the self-diffusion diffusion coefficient D has the form [17] $D = \frac{1}{3}\int_0^\infty \langle \mathbf{v}(0)\cdot\mathbf{v}(t)\rangle dt$ and the correlation function within the integral is of the same form as the first factor in eq.(12). It seems as if the diffusion coefficient is connected in some subtle way to the work done along a concentration gradient. A simplified Langevin-type treatment of black-body radiation [18] showed that the Planck constant could be directly related to various classical relaxation terms within the charged oscillator particles and although a first order approximation, it shows in principal the possible non-fundamental nature of the quantum and serves to encourage the pursuit of themes aimed at reducing QM to electrodynamics and mechanics without any further ad hoc assumptions. The differential equation considered was

$$m\ddot{X} + a\dot{X} + kX = 0 \qquad (13)$$

for these charged oscillators lining the blackbody (BB) cavity, with a combined electromagnetic and viscosity damping term

$a = \bar{\gamma} m$ where m is the mass of the electron and k the restoring force of the oscillators. The difference from standard Langevin analysis is that we consider this equation to hold up to time τ, the mean relaxation time, where the radiation from the cavity interacts with the wall enclosure lattice and charged particles to reconfigure the oscillator after this time τ. A key point in the argument was the observation or insistence that the Rayleigh-Jeans concept of equipartition was misconstrued and misunderstood; in our model,each element of frequency range belongs to a different oscillator and therefore different Hamiltonian type that could not be averaged in one lumped sum. A very basic analysis leads to a first order temperature independent Planck "'constant"' h relative to the oscillator properties as

$$h = \kappa 4c^3 \alpha \pi^3 N \tau^2 \qquad (14)$$

where $\alpha = m < X_o^2 > /2$; X_o is the amplitude of the oscillator; c is the speed of light; N is the number of oscillators inside the the BB cavity. Define $Q = \frac{e^2}{12\pi\varepsilon_0 c^3}$, k' the Boltzmann constant and $(k'T)^2\tau^3 m/(2Q) = <\gamma>^2$. Since τ varies inversely with temperature, we expect $<\gamma>$ to be a slowly varying function of temperature at around 300K. The average leakage per oscillator is $<<P>> = k'T <\gamma>$. Hence the unexpected outcome of this very approximate model was that a 2-D system of dipole oscillators would emit radiation as a power of approximately T^1 (for constant $<\gamma>$) rather than T^4 as is currently believed and practiced, where the $4th$ order power law expression, especially in radiation engineering has evolved into a sophisticated science.

Ref.[19] was a paper of far-reaching consequences which was unfortunately marred by wrong typesetting by the publisher in England with an apology and Erratum duly issued [20]; its content showed that the standard Liouville equation

which is the basic equation of dynamics used in both statistical mechanics and its quantum analogs to derive fundamental results does not have the purported solutions attributed to it from the continuum equation. For instance, the standard partition of the Hamiltonian leads to the elementary result in theorem form:

Theorem 1 *If the Hamiltonian H is partitioned as a linear functional of the coordinates* ***q*** *and the momenta* ***p*** *with no cross-terms as $H = K(p) + V(q)$ then each component of the divergence is zero where $div(\dot{p})_k = div(\dot{q})_k = 0$ for all indices k.*

From Theorem 1 the following obtains:

Corollary 1 *The general solution to the problem of partitioned Hamiltonian coordinates according to Theorem 3 is $\frac{\partial \dot{q}_k}{\partial q_k} = \frac{\partial \dot{p}_k}{\partial p_k} = 0$ for all k.*

The general solution to the problem of Corollary 1 *in Γ space* is therefore $q = \mathbf{C}t + \beta$ for the position coordinates and $\mathbf{p} = \mathbf{D}t + \gamma$ for the momentum coordinates where $\mathbf{C}$ and $\mathbf{D}$ are constant vectors, and t is the time coordinate. Since $\frac{\partial \rho}{\partial t} = -\mathbf{v}.\nabla\rho$, it follows that the phase density gradient is orthogonal to the velocity, and such a solution implies *equidensity* contours of ρ that are all parallel to the velocity vector, like a sheath enclosing a line. This result as it stands would not accord with the well known Gibbs canonical distribution assumption for equilibrium systems [21].

By viewing the situation stochastically, the following was derived and stated [19]:

Theorem 2 *It is possible to derive a stochastic equation having the form of the Liouville equation with form*

$$\left\langle \frac{\delta F}{\delta t} \Big|_{p,q} \right\rangle = -\nabla\rho.\mathbf{v} \qquad (15)$$

where $\rho \equiv F$ is a defined non-Liouville density.

At equilibrium, we infer $\left\langle \frac{\delta F}{\delta t} \Big|_{p,q} \right\rangle = 0 \Rightarrow -\nabla\rho.\mathbf{v} = 0.$

The work on electrochemistry derived and tested another type of chemical potential from basic thermodynamical definitions $\mu = \mu_F(e) + \varepsilon_{xc}$ [13] [eq.15] compared to the standard Seitz form μ_S used in advanced solid state theory [22,23], where $\mu_S = \varepsilon_o + d[n\varepsilon_{xc}(n)]/dn$ where ε_{xc} was the exchange-correlation energy of the electron; it was opined that the new form was more consistent with the preliminary and restricted-in-scope experimental result of observing how two electrodes of the same genus could show emf differences between them due to size effects by direct computations comparing the two types of chemical potentials where the electrochemical assumption has always been the constancy of the electrochemical potential of the electron in the substrate electrodes.

[C] Foundational studies in mechanics, quantum mechanics and radiation

Jesudason [24] concentrated on testing out the theoretical predictions in [25] of Fourier-like radiation flux terms emitted by a 2-D surface; it was found through preliminary experiment using a radiation thermal conductivity apparatus that 80% of the radiation was Fourier -like, but this was lowered for coiled systems where cavity radiation became more important. Small temperature differences could be detected which persisted over long time intervals (hours); whilst this might be due to experimental uncertainty and artefacts or cross effects, a theory was created to explain this phenomenon if this observation is indeed true; a completely new theory of

the Kirkhoff radiation law, together with other very fundamental ideas and alternatives to the Gibbs criterion for equilibrium and another definition for entropy based on coupling coefficients other than the Boltzmann constant was derived since the previous concepts all refer to a unique fixed temperature parameter for any equilibrium state. Ref. [26] is a broad study of the axiomatic foundations of quantum theory as well as a critique of the Heisenberg theory concerning uncertainty relations and also of wavemechanics. Let $v(A,B)$ to be a function space that is spanned simultaneously by the eigenfunctions of operator $\hat{A}$ and $\hat{B}$. Here, it is stated that the functions that span this space are functions of the *same* coordinate space. All the algebraic studies do not state this , and it is interesting that whenever "Heisenberg Uncertainty" obtains for certain operators, the coordinate spaces are usually restricted for some of the eigenfunctions and their associated operators in such a way that Heisenberg Uncertainty follows. In this work, a theorem was stated and proved [26] [theorem 3]:

Theorem 3 *If* $[\hat{P},\hat{Q}]=0$ *where* $\{\varphi_i\}\equiv v(P,Q)$ *is a complete (possibly nondegenerate) set of eigenfunctions without domain restriction, and* $[\hat{P},\hat{R}]=0$ *corresponds to the complete eigenfunctions* $\{\Psi_i\}\equiv v(P,R)$ *with the same conditions as* $\{\varphi_i\}$*, then* $\{\Psi_i\}$ *must be eigenfunctions of* $\hat{P}$ *and* $\hat{Q}$.

This result precludes the presence of Heisenberg Uncertainty due to the transitive relationship and therefore if Heisenberg Uncertainty is to be "saved", then another calculus focusing attention on the coordinate space must be invented to ensure that the operators are not transitive. An examination of the Schrödinger wave theory from first principles shows that the coordinates used in the wavefunction is identical to that of the particle coordinates, so that no Heisenberg Uncertainty is implied in the sense of specific common coordinates. Interestingly, Schrödinger in his second communication of 1927

admits the novelty of the variation that he wrote to arrive at his wave mechanics, namely

$$\delta \int (H - E) = 0 \qquad (16)$$

where H and E are the Hamiltonian and energy; and $(H - E)$ is already a constant; more recently relative to 1927, such related variations, called "'trivial"' have been applied to problems in irreversible thermodynamics [8]. In these trivial variational problems, a potential Φ was constructed as $\Phi = \sum \sum a_{ij}\varphi_{ij}$ for all coupled flows, where $\delta \int J_i \mathbf{dR} = 0$ and where for instance

$$\Phi_{J_\alpha} = \frac{\partial}{\partial Y_\alpha} \sum_{i}^{\infty} \sum_{j}^{\infty} D_{ij} Y_\alpha^i Y_\beta^j$$

and $J_{\alpha,x} = \frac{\partial \Phi_{J_\alpha}}{\partial x}$. The reciprocity relations were recovered for this construct.

Jesudason [5,6] analytically disproved the century and a half or perhaps earlier belief in time-reversal symmetry which became a cornerstone in not just mechanics and statistical mechanics (e.g. Onsager's reciprocity relations) but of Quantum Mechanics (CPT theory). A cautionary note must be made here. There are several definitions of "time reversal" invariance, some of which are mathematically consistent [27,28] and others which are not. The work here only examines those definitions in Physics which are not consistent, such as that described by van Kampen [29] and others in the physical sciences [30].

The surprising result related to the Planck radiation law with oscillator emission $P = \gamma' k' T$ described in Sec. **[B]** was experimentally checked using a modified thermal conductivity apparatus that could measure radiation fluxes .

Even without these conjectures, by averaging over different frequencies, a different expression for the radiancy [24] (of great importance to astronomy and other imaging techniques) E_{bv} was derived as

$$E_{bv} = (2\pi h\nu^3/nc^2)[exp(h\nu/n^3k'T) - 1]^{-1} \quad (17)$$

as contrasted to the standard expression

$$E_{bv} = 2\pi h\nu^3 n^2/c^2)[exp(h\nu/k'T) - 1]^{-1} \quad (18)$$

where k' is the Boltzmann constant. The development of the generalization of the Kirchoff radiation laws are to be found in [24, eqns. 11 and 12] and has the form

$$P_e^{C_j}(-\mathbf{k}.\alpha,\beta = T_{C_j}k_{C_j}/a^{C_j}(\mathbf{k},\alpha,\beta) = P_i(\mathbf{k},\alpha,\beta)$$

$$= f_A(\beta) \quad (19)$$

or

$$P_e^{C_j}(-\mathbf{k}.\alpha, T_{C_j}k_{C_j}/f_A(\beta) = \varepsilon_{C_j} = a^{C_j}(\mathbf{k},\alpha,\beta) \quad (20)$$

where The P's are the emission in direction $\mathbf{k}$, a^{C_j} the absorbance at the same temperature T_{C_j}, P_i the incident radiation of the standardized radiator A which is a function of $\beta = T_{C_j}k_{C_j} = kT$ only, so that $P_i = f_A\beta$ with f_A the incident radiation factor. The entropy increment must have the form $dS' = dQ/(k(\mathbf{R})T = dQ/\beta$ and is a perfect differential i.e. $\oint dS' = 0$.

[D] Molecular dynamics and NEMD simulations of complex systems

Description of thermomechanically coherent reacting dimer

The dimeric particle reaction studied is

$$2A \rightleftharpoons A_2 \quad (21)$$

above the supercritical regime of the LJ fluid with $T^* = 8$ at $\rho = 0.7$ with the formation of the dimer at $r_f = 0.85$ and $r_b = 1.20$ for the point of breakdown. The details of this model are in [31]. Thermomechanical-coherence is connected to the rotational energy work and its changes as the bond length changes in value from the time of formation to the point of breakdown. The total work done is connected to the free energy of formation of the dimer; clearly, the moment of inertia features in the calculations.

$$\mathrm{A_n} + \mathrm{A_m} \leftrightarrow \mathrm{A_{m+n}} \tag{22}$$

a general scheme is depicted in Fig. 1 with the appropriate coordinates. The simulation result reported here is when $n = m = 1$ for a simple dimer reaction.

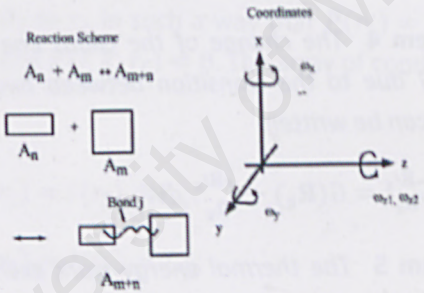

Fig. 1: Diagrams depicting the rotational axes and "'bond"' formation j due to internal forces.

For rotational motion, consider an element of thermal energy due to rotation about the given (z) axis given by the form

$$E_{TY} = E_{TY}(T, I_z, TH = \mathrm{rotn, z}) \tag{23}$$

For rotational motion, the mechanical, non-thermal rotational energy (denoted $E_{Mech,Rot,z}(I(\mathbf{R_z}), \boldsymbol{\Omega})$ would suffer loss δE_{Mech} if $\delta I_z > 0$ because of conservation of angular momentum and

the net work dW that would have to be done to enable energy balance for an ideal centrifugal heat engine is

$$dW_z = \left(dE_{TY}(TH = Rotn, z) - dE_{Mech,Rotn,z}\right) \quad (24)$$

I will always refer to the moment of inertia with subscripts referring to the species type. For instance, if only the z coordinates are involved then a simplified expression is

$$dW_{G,z} = \left(\frac{\partial E_{TY}(TH=Rotn,z)}{\partial \mathbf{R_z}} \cdot \mathbf{dR_z} \quad (25)\right.$$

$$\left. -\frac{\partial E_{Mech,Rotn,z}(TH = Rotn, z)}{\partial \mathbf{R_z}}|_{T.E.} \cdot \mathbf{dR_z}\right) = -\mathbf{F_{I,z}} \cdot \mathbf{dR_z}$$

where subscript $T.E$ denotes a pathway along that of thermal equilibrium, $\mathbf{F_I, z}$ is the resultant internal force.

Furthermore the following were proved:

Theorem 4 *The change of the Gibbs energy between two states ΔG due to the transition between two coordinate points $\boldsymbol{R_z}, \boldsymbol{R'_z}$ can be written*

$$\Delta G_{\mathbf{R_z}}^{\mathbf{R'_z}} = G(\mathbf{R_z}) + \int_{\mathbf{R_z}}^{\mathbf{R'_z}} dW_{G,z} \quad (26)$$

Theorem 5 *The thermal energy-work exchange $\Delta W_{r_1}^{r_2}$ between internuclear distances r_1 and r_2 is given by*

$$\Delta W_{r_1}^{r_2} = -\left(\overline{E}_{rot}\right)\ln\left(\frac{I(r_1)}{I(r_2)}\right) \quad (27)$$

Theorem 6 *The total change of the free energy about the bond trajectory ΔG_{mol} is given by*

$$\overline{W_{rf}} = \int_{r=0}^{r_b} \Delta W_{r_f}^{r_2} P(r_2) dr_2 = \Delta G_{mol}. \quad (28)$$

where $P(r_2)$ is a probability density function for the internuclear distance r_2. Finally some approximations may be derived. Some exact expressions will be presented later. If the work done is approximately equal to the rotational energy

dissipation, then $\delta U \approx \delta w + \delta q = 0$ or $\delta q \approx \delta w$, or $T\delta S \approx -\delta w$ or by integration $T\Delta S_{r_f}^{r_2} \approx \Delta W_{r_f}^{r_2}$ and so

$$T\langle \Delta S \rangle = T \int_{r=0}^{r_b} \Delta S_{r_f}^{r_2} P(r_2) dr_2 \approx \overline{W_{rf}} \qquad (29)$$

or

$$\langle \Delta S \rangle \approx \left(\frac{W_{rf}}{T} \right) \qquad (30)$$

At present, the form of P is not available, since the simulation program developed did not anticipate the need for this distribution, but it will be included in future investigations for the years ahead. The several scenarios are listed below for the above dimer reaction:

1. the molecule is formed at r_f and then traverses instantaneously to r_b in such a way that $P(r_2) = \text{constant} = 0$ except for r_b and $P(r < r_f) = 0$. The array of conditions may be written

$$I(r_1) = I(r_f) = I_{r_f},$$

$$I(r_2) = I(r_b) = I_{r_b},$$

$$\overline{W_{r_f}}^{(1)} = -2(\overline{E}_{rot}) \ln \left(\frac{I_{r_f}}{I_{r_b}} \right) \qquad (31)$$

The parameters are $r_f = 0.85, r_b = 1.20, I_f = 0.36125, I_b = 0.720$. For the 2 rotational modes at $T^* = 8, \overline{E}_{rot} = 4.0$ for classical systems, so that (31) yields $\overline{W_{r_f}}^{(1)} = 0.6862T^*$

2. since ΔG^o $(T^* = 8)$ is known from the simulations, we can adjust $I(r_2)$ ($I_{r_1} = I_{r_f}$ is fixed) so that there is exact coincidence at ΔG^o $(T^* = 8)$; this occurs when $r_f = 1.1539$ (instead of 1.20) and $I(r_b) = 0.6656$ where r_f and I_f are as in 1. above.

The $\overline{W_{r_f}}$ function, denoted in this instance $\overline{W_{r_f}}^{(2)}$ is from (42) $\overline{W_{r_f}}^{(2)} = 0.61110T^*$

3. Here we choose $I_{rat} = -\ln\left(\frac{I_{r_f}}{I_{r_b}}\right) = 0.50$, where $\left(\frac{I_{r_f}}{I_{r_b}}\right) = 0.60653$ and the W_{r_f} function in this case is $W_{r_f}^{(3)} = 0.50T^*$

Thus, for thermo-mechanical coherent systems, as defined in (28), we have

$$\Delta G^o(T) = \overline{\Delta G}(T) = \Delta G_{1\to 1^*} + \int_0^{r_b}\left(\int_{1^*}^{r_2} dG\right)P(r_2)dr_2$$

or

$$\Delta G^o(T) = \Delta G_{1\to 1^*} + \overline{W_{rf}} \tag{32}$$

with $\overline{W_{rf}}$ defined as in (28). In general, however,

$$\Delta G^o(T) = \Delta G_{1\to 1^*} + \int_0^{r_b}\left(\int_{1^*}^{r_2}(dH - TdS)\right)P(r_2)dr_2. \tag{33}$$

Eq. (32) will be considered in detail in the next section. We also define the following energy term for the two cases that we may encounter:

$$\overline{W_{rf}}' = \begin{cases} \overline{W_{rf}} \text{ from (28) if system is thermomechanically coherent,} \\ \text{otherwise we set} \\ \int_0^{r_b}\left(\int_{1^*}^{r_2}(dH - TdS)\right)P(r_2)dr_2 \end{cases} \tag{34}$$

Estimates of $\Delta G^o(T)$

From (32), and (31),we derive

$$\Delta G^{0(1)}(T) = \Delta G_{1\to 1^*} + \overline{W_{rf}}^{(1)} = 17.5153 + 0.6862T^* \tag{35}$$

$$\Delta G^{0(2)}(T) = \Delta G_{1\to 1^*} + \overline{W_{rf}}^{(2)} = 17.5153 + 0.61110T^* \tag{36}$$

$$\Delta G^{\,0\,(3)}(T) = \Delta G_{1\to 1^*} + \overline{W_{rf}}^{(3)} = 17.5153 + 0.500T^* \qquad (37)$$

Results From Estimates

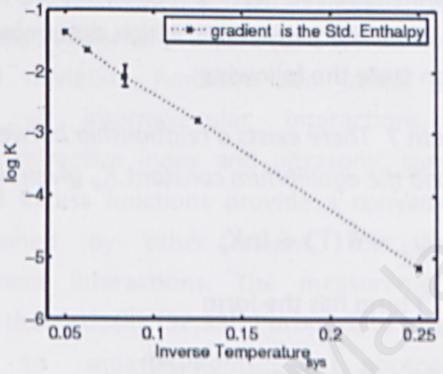

Fig. 2: Linear Plot of $\ln K_e \;\; vs \;\; 1/T^*$

From the above we can derive estimates for the standard Gibbs free energy, entropy and enthalpy of the reaction.

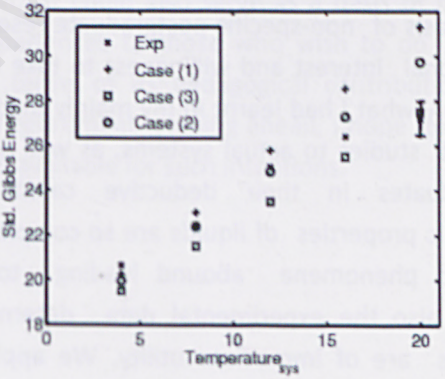

Fig. 3: Plots of the estimation of the standard Gibbs' energy for the three cases discussed in the text together with the simulation results.

Some other theorems immediately follow from the probability distribution.

Basis for Hammet-Taft-Curtin Relations

If we admit that simple collision theory (SCT) or the quantum version due to Eyring leads to Arrhenius type equations for elementary reactions which determines the rate law then we can state the following:

Theorem 7 *There exists a relationship between the rate constant* $k_{r,i}$ *and the equilibrium constant* K_e *given by*

$$\ln k_{r,i} = B(T) + \ln K_e \qquad (38)$$

where the $B(T)$ term has the form

$$B(T) = \ln\left[A'_i(T)\exp\frac{\overline{W_{rf}}'}{kT}\right]. \qquad (39)$$

and [31] [eq.65-67] provides both a proof of the above and its equivalence to the Taft-Hammett.

[E] Liquid-state laboratory for post-graduate opportunies in independent research.

From about 2010, a basic liquid state laboratory was set up as a basis of non-specific postgraduate research based on their personal interest and willingness to take risks. I also wished to apply what I had learnt in my mainly theoretical and computational studies to actual systems, as well as challenge the postgraduates in their deductive capabilities. The thermodynamic properties of liquids are so complex that new theories and phenomena abound leading to abundant explanations; also the experimental data determined from measurements are of immediate utility. We apply different experimental techniques to determine multicomponent (usually binary) mixture data such as densities (ρ), ultrasonic speeds (u), and refractive indices (nD), viscosities, (η) of binary

mixtures, including those of their pure liquids, are measured over the entire composition range at different temperatures. From the experimental data, the excess molar volume (VE), deviations in isentropic compressibility (Δks), deviations in molar refraction (ΔRm), deviations in refractive index (ΔnD), deviations in ultrasonic speed, (Δu), deviations in viscosity ($\Delta\eta$) and deviations in internal pressure (ΔPi) were calculated. These excess and deviation functions are useful tool for the elucidation of intermolecular interactions. Volumetric, viscometric, refractive index and ultrasonic speed and their derived and excess functions provide a convenient tool, not easily obtained by other means, for the study of intercomponent interactions. The measurements are also rationalized theoretically [32,33]. I propose to extend this basic laboratory to measurements in photoelectric and photochemical energy systems.

CONCLUDING REMARKS

The work cursorily described above covers part of a much wider area which would obviously require further consolidation. It could also serve as a basis of relating these research experiences to those who wish to do independent research in terms of its pedagogical contribution. With the prospects of retirement looming ahead, I hope to use some of the free time available for such intentions.

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ACKNOWLEDGEMENTS

I am deeply grateful to my parents, relatives and friends, in particular my mother Ruby Selvaranee Saravanamuthu (9.3.1926-21.7.2015) for showing a lifelong example of faith in charity, endurance and incessant labour, qualities that I too had to cultivate to pursue my chosen work and existential trajectory. I am also grateful in one sense to University of Malaya for providing - until very recently some might say - academic space and freedom of inquiry despite the encroaching regimentation of globalism, with its universalism that cannot take into account the idiosyncrasies of peoples and cultures. Last but not least, to all my colleagues, past and present at the Department of Chemistry, UM who presented an optimistic predisposition whenever all seemed rather dark and gloomy, I cannot thank you enough.

CURRICULUM VITAE

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EDUCATION PARTICULARS

BA, 1980 (Queens' University of Cambridge, England)
post BA research (Chemistry Depart., Univ. of Malaya under Prof. T.K. Lim, registered as MSc candidate)
MA, 1982 (University of Cambridge, England)
PhD, 1986 (Studies in Thermodynamics, Major Professor Darwin W. Smith) Chemistry Department, University of Georgia, USA

EMPLOYMENT EXPERIENCES

Post-doctoral fellow, Montana State University, 1987-1989
University of Malaya, 1989 – Lecturer
University of Malaya, 2000 – Associate Professor
University of Malaya, 2008 – Professor

SELECTED RECENT ACADEMIC COURSE EXPERIENCES

(Based on gaining experience in research pedagogical development)

1 Computer Aided Drug Design (CADD 2016)
30/10/2016 -02/11/2016

2 Haddock Workshop Information-driven Modelling of Biomolecular Complexes, University of Cagliari, Sardinia, Italy
26/05/2016 - 01/06/2016

3 Wein2009: hands On Workshop on the Wien2k Package, Pennsylvania State University
22/06/2009 -27/06/2009

4 Theoretical Chemistry Workshop, USM, Penang
10/05/2006 -20/05/2006

5 Free Fluid-phase-thermodynamics and Cosmo-RS Couse, University Of Regensburg, Germany
09/10/2011 -15/10/2011

SELECTED MAINLY RECENT RESEARCH VISITS FOR BUILDING UP EXPERTIZE AND CREATING POSSIBLE LINKAGES

1 SABBATICAL V. UNIV. OF CAGLIARI, CAGLIARI, SARDINIA, ITALY
I spent my apparently last sabbatical in Cagliari with Prof. Francesca Mocci to study deep eutectic solvent liquid systems.
20/01/2016 -19/08/2016

2 DFT CALCULATIONS ON CHEMICAL SYSTEMS, NATIONAL CHEMICAL INSTITUTE, SLOVENIA
I visited the place to study bio-organic reaction with Prof Janez Mavri, where we hope to complete work on Curcumin reactions
24/07/2014 -12/09/2014

3 SABBATICAL IV. QUEEN'S UNIVERSITY BELFAST, UNITED KINGDOM BELFAST, U.K.
I was located in the Atomistic Simulation Centre headed by Prof Jorge Kohanoff to study MD simulation of MOF lattices with ionic liquid insertions
01/09/2012 -31/07/2013

4 SABBATICAL III (B). UNIVERSITY OF STOCKHOLM, ARRHENIUS LABORATORY, STOCKHOLM, SWEDEN
Study of charged systems with Profs. Aatto Laaksonen and Alexander Lyubartsev
01/06/2007- 15/12/2007

5 SABBATICAL III (A). HUT, HELSINKI FINLAND
Sabbatical to study molecular dynamics of charged systems with Mikko Kartunen
01/01/2007 -31/05/2007

6 VISIT TO UNIV OF MAINE, ORONO, MAINE, USA
Visit to eminent Prof. Jay Rasaiah to understand nature of the liquid state better and to suggest research collaboration
01/06/2006 -30/07/2006

7 LECTURE AT POLISH ACADEMY OF SCIENCE WARSAW
Visit to Polish Academy of science and delivery of lecture entitled "The Clausius Inequality: Implication for Non-Equilibrium Thermodynamic Steady States with NEMD Corroboration using a Dimeric Chemical Reaction"
15/11/2004-15/11/2004

8 RESEARCH VISIT TO SAINT PETERSBURG STATE UNIVERSITY, PETERGOFF, ST. PETERSBURG, RUSSIAN FEDERATION
Visit to Dr. Sergey Lukianoff, Chemistry Department, Saint Petersburg State University to study MPI methods and charged systems.
01/04/2003-01/06/2003

9 SABBATICAL II. INSTITUTE OF PHYSICAL CHEMISTRY NTNU, TRONDHEIM, NORWAY TRONDHEIM, NORWAY
I spent over 9 months there to acquaint myself with NEMD methods to study nonequilibrium thermodynamics simulation using the method of Bjorn Hafsjold
14/12/2000- 13/10/2001

10 SABBATICAL I. NATIONAL CHEMICAL INSTITUTE, SLOVENIA
Sabbatical visit to study Monte Carlo methods in simulations, centering on Hard-disk potential systems
04/12/1994 -31/08/1995

PUBLICATIONS

SELECTED BOOKS & CHAPTERS IN BOOKS

Books

Jesudason, C.G. 1996. Primary Abortion (University of Malaya Press, 1996, ISBN 983-99676-1-4) (Non-ISI/Non-SCOPUS)

Jesudason, C.G. 1992. Words from a Teleprinter Poem Written 1980-81. Kuala Lumpur: Alethia Enterprises. ISBN 983-99676-0-6 (Non-ISI/Non-SCOPUS)

Chapters in Book

Stefan, E. and Tapio W. (2008). Solving a dynamic separation problem using MINLP techniques. *Appl Numer Math*, *58*, 395-406. [MR2397945] published in Mathematical Reviews (AMS).

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Jesudason, C.G. (1998). An aspect of Heisenberg uncertainty and de Broglie waves in frontiers in quantum physics, p. 245. Verlag: Springer. (SCOPUS-Indexed).

SELECTED PUBLICATIONS IN JOURNALS AND PROCEEDING COLLECTIONS

Nabi, A., Yau, C. K. and Jesudason, C. G. (2016). Investigation of Molecular Interactions in Binary Mixtures (Dichloromethane + Aliphatic Alcohols) at T= (298.15 to 308.15) K: Experimental, ERAS Analyses and COSMO-RS Predictions. *Journal of Molecular Liquids*, *224*, 551-561.

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Yau, C.K., Nabi, F. and Jesudason, C.G. (2015). Ultrasonic Speeds, Refractive Indices, and Densities of Dimethoxymethane + Aliphatic Alcohols (C1-C4) at (298.15 and 303.15) K with COSMO-RS and ERAS analyses. *Mol Liquids*, *212*, 79-89.

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Rosli, N.A., Kassim, H.A., Jesudason, C.G. and Shrivastava, K.N. (2009). DFT Calculation of Vibrational Frequencies in Clusters of Fe and As Atoms. *AIP Conference Proceedings*, *1169*, 256.

Ling, L.L., Jesudason, C.G. and Shrivastava, K.N. (2009). Computerized Simulation of Magnetoresistance Random Access Memory Material. *AIP Conference Proceedings*, *1169*, 279.

Jesudason, C.G., Lyubartsev, A.P. and Laaksonen, A. (2009). Conformational Characteristics of Single Flexible Polyelectrolyte Chain. *Eur. Phys. J.E. Soft Matter*, *30*(4), 341-350.

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Jesudason, C.G. (2007). Model Hysteresis Dimer Molecule II: Deductions from Probability Profile due to System Coordinates. *Journal of Mathematical Chemistry*, *42*(4), 893-908.

SELECTED AWARDS AND RECOGNITIONS

No	Name of Award	Awarding Institution	Year Awarded	Level
1	Listing in Marquis' Who is Who (from 2000) Who's Who in the World (2006, 2008), Who's Who in Asia (2007)	Marquis bibliography services, USA	2016	International
2	Guest Editor for special issue "Modeling and Analysis in Thermodynamics and Heat Transfer"	Hindawi Publications	2015	International
3	Citation in Malaysia: Who's Who In The Civil Service: The Steel Backbone of The Government- Creme De La Creme	Kasuya Management Sdn Bhd Publication	2015	National
4	Certificate of Excellence	University of Malaya	2012	National
5	Elected Member of International Organizing committee, ICPPAA 2010 World Congress; 8th International Conference on Mathematical Problems in Engineering, Aerospace and Sciences	ICNPAA	2009	International
6	Khidmat Setia 20 Award	University of Malaya	2009	National
7	UMRG grant	University of Malaya	2009	University
8	Chairman of Session, Computation Methods and Applications-1, ICDSA5 , Atlanta, Ga, USA, 2007	International conference ICDSA_5, Atlanta, U.S.A.	2008	International

9	Entry in Dictionary of International Biography 2008 Cambridge Blue Book (a selection of the best scientists globally in their respective fields)	International Biography Centre, Cambridge, England	2008	International
10	FRGS grant	MOSTI (Government of Malaysia)	2008	National
11	PJP University Grant	University of Malaya	2008	University
12	PJP Research Grant RM 8,000	University of Malaya	2007	University
13	Bronze medal (Expo 2006 exhibition for fundamental research)	University of Malaya	2006	National
14	Penghargaan Persatuan Juruteknologis Makmal Universiti Malaya	University of Malaya	2006	University
15	Chairman of Session, Mathematical Methods 4, 19/Sept/2005, ICAAM 2005 International conference on mathematical methods, Rhodes, Greece	ICNAAM 2005	2005	International
16	Scholarship to decentralized renewable energy systems seminar and conference	Madrid (AECI, FIIAPP & CIEMAT)	2003	International
17	IRPA grant, RM198,000	MOSTI, Government of Malaysia	2003	National
18	PJP Grant, RM26,000	University of Malaya	2001	University

19	Preprint pioneer certificate- for first 1000 preprints sent to preprint server	Chemweb, United Kingdom	2000	International
20	T.W.A.S. research award	Third World Academy of Science	1999	International
21	Post Doctoral Fellowship	Montana State University, Bozeman	1986	International
22	University Teaching Assistant Award	University of Georgia	1985	International
23	University Teaching Assistant Award	University of Georgia	1983	International
24	Stipend to attend Cambridge University	Dorset County Council	1977	International
25	Scholarship	Bryanston Public School (England)	1974	International

PROFESSIONAL AFFILIATION/MEMBERSHIP (selection)

No	Organization	Role	Start date	Level
1	American Chemical Society	Member	2009	International
2	Institut Kimia Malaysia	Associate Member	2008	National/ International
3	IFNA-Int. Fed. Nonlinear Analysts	Member	2008	International
4	Institut Fizik Malaysia	Life member/Council Member	1989	National/ International